

chain nodes :
1 10 11 12 13 14 15 16 17 19
ring nodes :
3 4 5 6 7 8
chain bonds :
1-3 1-12 5-11 8-10 12-19 13-14 13-15 13-17 16-19
ring bonds :
3-4 3-8 4-5 5-6 6-7 7-8
exact/norm bonds :
1-3 1-12 3-4 3-8 4-5 5-6 5-11 6-7 7-8 8-10 12-19 13-14 13-15 13-17 16-19
G1:C,N
G2:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu,OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,CHO,[*1]

Match level :
1:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:CLASS 11:CLASS 12:Atom
13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:Atom
Generic attributes :
12:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic
19:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

10/623640

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *

SESSION RESUMED IN FILE 'CAOLD' AT 16:58:36 ON 16 JUN 2004

FILE 'CAOLD' ENTERED AT 16:58:36 ON 16 JUN 2004

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	183.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.08

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	183.39

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.08

FILE 'REGISTRY' ENTERED AT 16:58:44 ON 16 JUN 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3

DICTIONARY FILE UPDATES: 15 JUN 2004 HIGHEST RN 693773-36-3

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d his

(FILE 'HOME' ENTERED AT 16:50:31 ON 16 JUN 2004)

FILE 'REGISTRY' ENTERED AT 16:50:39 ON 16 JUN 2004

L1 STRUCTURE UPLOADED
L2 1 S 2,5-PIPERAZINEDIONE/CN
L3 0 S 46.383
L4 524029 S 46.383/RID
L5 0 S L1 SAMPLE SUB=L4
L6 131 S L1 FULL SUB=L4

FILE 'CAPLUS' ENTERED AT 16:54:06 ON 16 JUN 2004

FILE 'CAPLUS' ENTERED AT 16:54:30 ON 16 JUN 2004

10/623640

L7 3 S L6

FILE 'CAOLD' ENTERED AT 16:55:25 ON 16 JUN 2004

L8 0 S L6

FILE 'REGISTRY' ENTERED AT 16:58:44 ON 16 JUN 2004

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	183.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.08

FILE 'CAPLUS' ENTERED AT 16:58:59 ON 16 JUN 2004

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FILE COVERS 1907 - 16 Jun 2004 VOL 140 ISS 25

FILE LAST UPDATED: 15 Jun 2004 (20040615/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 16:50:31 ON 16 JUN 2004)

FILE 'REGISTRY' ENTERED AT 16:50:39 ON 16 JUN 2004

L1 STRUCTURE UPLOADED
L2 1 S 2,5-PIPERAZINEDIONE/CN
L3 0 S 46.383
L4 524029 S 46.383/RID
L5 0 S L1 SAMPLE SUB=L4
L6 131 S L1 FULL SUB=L4

FILE 'CAPLUS' ENTERED AT 16:54:06 ON 16 JUN 2004

FILE 'CAPLUS' ENTERED AT 16:54:30 ON 16 JUN 2004

L7 3 S L6

FILE 'CAOLD' ENTERED AT 16:55:25 ON 16 JUN 2004

L8 0 S L6

10/623640

FILE 'REGISTRY' ENTERED AT 16:58:44 ON 16 JUN 2004

FILE 'CAPLUS' ENTERED AT 16:58:59 ON 16 JUN 2004

=> s 16

L9 3 L6

=> d 17 1-3 bib abs

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2004:214115 CAPLUS

TI Small molecule biaryl FSH receptor agonists. Part 2: Lead optimization via parallel synthesis

AU Guo, Tao; Adang, Anton E. P.; Dong, Guizhen; Fitzpatrick, Dan; Geng, Peng; Ho, Koc-Kan; Jibilian, Charles H.; Kultgen, Steven G.; Liu, Ruiyan; McDonald, Edward; Saionz, Kurt W.; Valenzano, Kenneth J.; Van Straten, Nicole C. R.; Xie, Dan; Webb, Maria L.

CS Pharmacopeia, Inc., Princeton, NJ, 08543-5350, USA

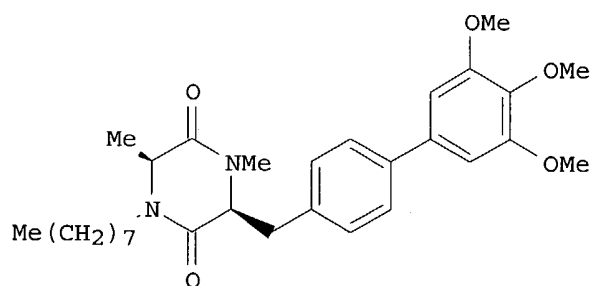
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(7), 1717-1720
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

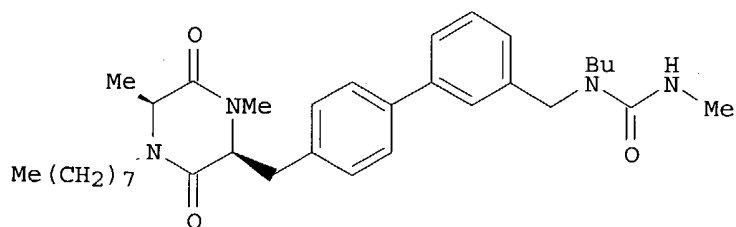
DT Journal

LA English

GI



I



II

AB Potent small mol. biaryl diketopiperazine FSH receptor agonists such as I (EC₅₀=13 nM) and II (EC₅₀=1.2 nM) were discovered through the design, synthesis and evaluation of three biaryl diketopiperazine optimization

10/623640

libraries with over 300 compds. These libraries were prepared via solid-phase parallel synthesis using a cyclization-release method.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:511150 CAPLUS

DN 139:85377

TI Preparation of substituted diketopiperazines as oxytocin antagonists

IN Borthwick, Alan David; Hatley, Richard Jonathan; Hickey, Deirdre Mary
Bernadette; Liddle, John; Livermore, David George Hubert; Mason, Andrew
Mcmurtrie; Miller, Neil Derek; Nerozzi, Fabrizio; Sollis, Steven Leslie;
Szardenings, Anna Katrin; Wyatt, Paul Graham

PA Glaxo Group Limited, UK; et al.

SO PCT Int. Appl., 90 pp.

CODEN: PIXXD2

DT Patent

LA English

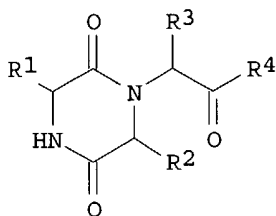
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053443	A1	20030703	WO 2002-EP14823	20021220
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
	CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
	GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
	LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,				
	PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT,				
	TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ,				
	MD, RU, TJ, TM				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,				
	CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,				
	PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,				
	NE, SN, TD, TG				

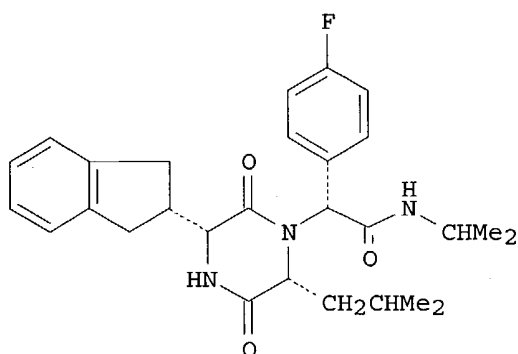
PRAI GB 2001-30677 A 20011221

OS MARPAT 139:85377

GI



I



II

AB Diketopiperazines I [R1 = optionally hydroxylated alkyl, cycloalkyl, benzocycloalkyl; R2 = Alkyl, alkoxyalkyl, alkylthioalkyl, dialkylaminoalkyl, cycloalkylalkyl, 5-6-membered heterocycle containing a single O, S, NMe, NEt; R3 = (un)substituted Ph, heteroaryl, bicyclic, heterobicyclic; R4 = OH, acyloxyalkoxy, (un)substituted NH2] were prepared for treating or preventing diseases or conditions mediated through the action of oxytocin (no data). Thus, the piperazinedione II was obtained by 4-component reaction of H-D-Leu-OMe.HCl, 4-FC6H4CHO, Me2CHNC, and N-tert.-butoxycarbonyl-D-indanylglycine.

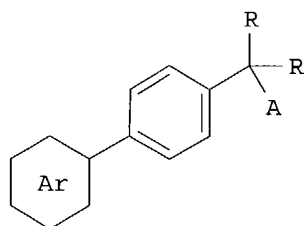
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:695961 CAPLUS
DN 137:216961
TI Preparation of bisaryl derivatives having FSH receptor modulatory activity
IN Guo, Tao; Ho, Koc-Kan; McDonald, Edward; Dolle, Roland Ellwood; Saionz, Kurt W.; Kultgen, Steven G.; Liu, Ruiyan; Dong, Guizhen; Geng, Peng; Adang, Anton Egbert Peter; Van Straten, Nicole Corine Renee
PA Pharmacopeia, Inc., USA
SO PCT Int. Appl., 167 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

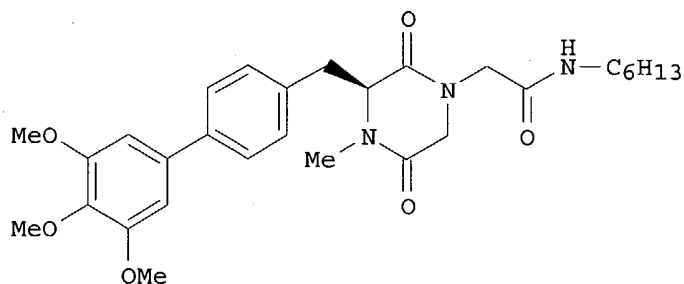
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002070493	A1	20020912	WO 2002-US3777	20020118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				

10/623640

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP 1351941 A1 20031015 EP 2002-717403 20020118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRAI EP 2001-200194 A 20010119
WO 2002-US3777 W 20020118
OS MARPAT 137:216961
GI



I



II

AB Title compds. I [R,R = H/H, O, H/Me, H/OH, H/CN; A = pyridazindione, etc.; Ar = (un)substituted phenyl] were prepared For example, a photolabile-supported 1-hexylamine derivative was acylated with (3S)-1-carboxymethyl-3-(4-iodobenzyl)-4-methyl-2,5-dioxopiperazine (preparation given) followed by coupling of the resulting aryl iodide with 3,4,5-trimethoxybenzeneboronic acid (DME/EtOH, Pd2(dba)3, Ph3As, CsF). The resulting resin was irradiated at 365 nm at 50° (MeOH/TFA) to yield II. II had EC50 < 10 µM for the FSH receptor. I are useful in the treatment for the control of fertility, for contraception or for treatment of hormone-dependent disorders.

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 17 2 hitstr

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

IT 554447-22-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological

10/623640

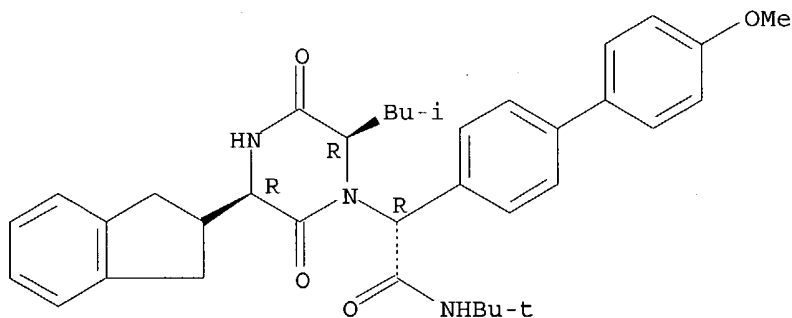
study); PREP (Preparation); USES (Uses)

(preparation of substituted diketopiperazines as oxytocin antagonists)

RN 554447-22-2 CAPLUS

CN 1-Piperazineacetamide, 3-(2,3-dihydro-1H-inden-2-yl)-N-(1,1-dimethylethyl)-
α-(4'-methoxy[1,1'-biphenyl]-4-yl)-6-(2-methylpropyl)-2,5-dioxo-,
(αR,3R,6R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> file caold

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

10.71

194.52

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-2.08

-4.16

FILE 'CAOLD' ENTERED AT 17:00:06 ON 16 JUN 2004

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> s l6

L10

0 L6

=>